Quantum Mechanics

Topics Covered

→ Black Body Radiation [Postulates of Quantum Mechanics]
→ Heisnberg's Uncertainity Principle
→ Wave Particle Duality [De-Broglie Hypothesis]
→ Matter Waves
→ Group and Phase Velocity
→ Wave Function [Properties and Physical Significance]

Why Quantum Mechanics?

It is required to explain the behaviour of matter and radiation at atomic level (when system size is below 10^{-9} m), where classical physics fails. Classical physics fails to explain-

→ Spectrum of blackbody radiation
→ Photoelectric effect
→ Wave-particle duality
→ Quantized or discrete energy

So, quantum mechanics becomes essential for accurately describing and predicting microscopic phenomenon.

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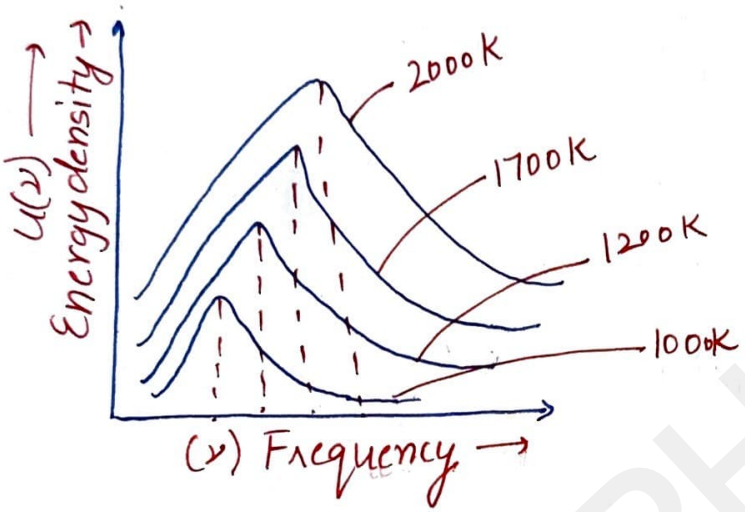
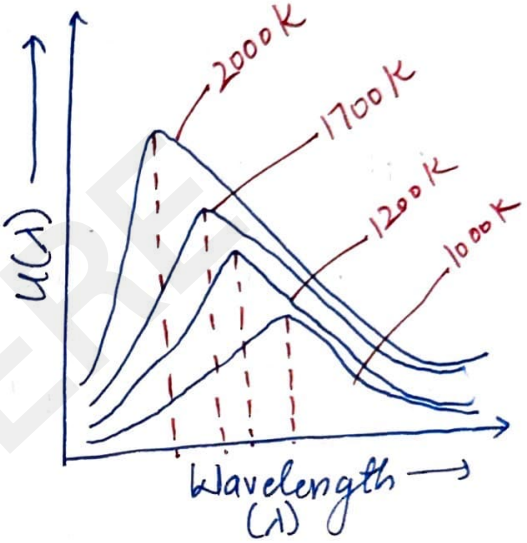
Black-Body Radiation

Definition :- A body that completely absorbs radiations of all wavelengths incident on it is referred as blackbody.

Spectrum :-





Postulates of quantum mechanics [Planck's radiation law]

Max Planck in 1900 introduced the quantum theory of radiation and explained distribution energy in blackbody radiation spectrum. He postulated -

① An oscillator cannot have any arbitary value of energy but can have only discrete energies as per following relation. $E = nh\nu$

where $n = 0, 1, 2 \ldots$, ν is frequency of oscillator and h is Planck's constant.

② The oscillator can emit or absorb energy in form of packets of energy ($h\nu$), but not continuously. So that -

$$\Delta E = \Delta n h\nu \quad \text{or} \quad E_2 - E_1 = (n_2 - n_1) h\nu$$

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Based on these postulates, the Planck's radiation law is given as-

$$u(\nu)d\nu = \frac{8\pi h}{c^3}\frac{\nu^3 d\nu}{e^{h\nu/k_BT} - 1} \quad \rightarrow (1)$$

or

$$u(\lambda)d\lambda = \frac{8\pi hc}{\lambda^5}\frac{d\lambda}{e^{\frac{hc}{\lambda k_BT}} - 1} \quad \rightarrow (2)$$

Wien's Law

Using the thermodynamic physics, the formula for blackbody spectrum was given as-

$$u(\lambda)d\lambda = \frac{8\pi hc}{\lambda^5} e^{\frac{-hc}{\lambda k_BT}} d\lambda$$

$8\pi hc = C_1$ and $\frac{hc}{k_B} = C_2$

$$\Rightarrow \boxed{u(\lambda)d\lambda = \frac{C_1}{\lambda^5} e^{-\frac{C_2}{\lambda T}} d\lambda} \quad \rightarrow (3)$$

⇒ Applicable only at low wavelength and high frequency.

Wein's law from Planck's law

We have, in Planck's formula $e^{\frac{hc}{\lambda k_BT}}$ in denominator, see equation (2)

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When, wavelength is low, $\frac{hc}{\lambda K_B T}$ becomes very large, so $e^{\frac{hc}{\lambda K_B T}}$ is a large quantity and we ignore 1 in comparison in equation 2-

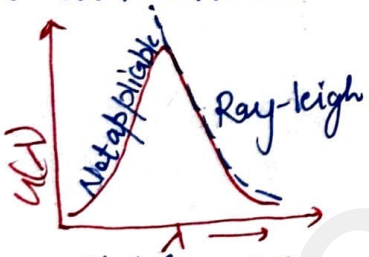
so we have,

$$u(\lambda)\,d\lambda = \frac{8\pi hc}{\lambda^5} \frac{d\lambda}{e^{\frac{hc}{\lambda K_B T}}}$$

which gives the Wien's law.

Ray-leigh and Jeans Law

There law was based on the idea that energy emitted is continuous. Based on this, they formulated



$$u(\lambda)d\lambda = \frac{8\pi K_B T}{\lambda^4} d\lambda \quad \rightarrow (4)$$

⇒ Applicable only at higher wavelength and lower frequency.

Rayleigh's law from Planck's formula

In Planck's formula in equation 2, $e^{\frac{hc}{\lambda K_B T}}$ is in denominator, since Rayleigh's law is applicable only at higher wavelength, the factor $\frac{hc}{\lambda K_B T}$ becomes very small. Hence this can be written as -

$$e^{\frac{hc}{\lambda K_B T}} = 1 + \frac{hc}{\lambda K_B T} + \dots \quad [\text{We ignored higher orders}]$$

$$\left[e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots\right]$$

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Substituting in equation 2-

$$u(\lambda)\,d\lambda = \frac{8\pi hc}{\lambda^5}\,\frac{1}{\left[1+\frac{hc}{\lambda k_B T}-1\right]}\,d\lambda$$

$$u(\lambda)\,d\lambda = \frac{8\pi k_B T}{\lambda^4}\,d\lambda$$

which is Rayleigh's law.

Heisnberg's Uncertainity Principle

It states that it is impossible to determine simultaneously the exact position and momentum of a small moving particle. Mathematically it is represented as-

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$

[Δx is uncertainity in position, Δp is uncertainity in momentum]

$$\Delta E \cdot \Delta t \geq \frac{h}{4\pi}$$

[ΔE is unartainity in energy, Δt is uncertainity in time]

$$\Delta J \cdot \Delta \theta \geq \frac{h}{4\pi}$$

[ΔJ is uncertainity in angular momentum, $\Delta\theta$ is uncertainity in angle]

⇒ A particle is represented by a wave packet, formed by superposition of many waves. To confine the particle into a small region of space, waves with a wide range of wavelengths must be confined. This spread will lead to an uncertainity in momentum

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⇒ If we define momentum, position will become uncertain.

Applications of Uncertainity Principle

① Non-existence of electrons in the nucleus.

From Heisnberg's uncertainity principle we have,

$$\Delta x . \Delta p = \frac{h}{4\pi}$$

let us suppose that electrons exist inside the nucleus. Now, the maximum uncertainity will be of order of size of nucleus, so $\Delta x \simeq 10^{-14} m$

Hence we have $10^{-14} . \Delta p = \frac{h}{4\pi}$

$$\Rightarrow \Delta p = \frac{6.626 \times 10^{-34} \text{ J-s}}{4 \times 3.14 \times 10^{-14}}$$

$$= 0.527 \times 10^{-20} \text{ kg m/s}$$

We know that kinetic energy, $E = \frac{1}{2} mv^2 = \frac{(mv)^2}{2m} = \frac{p^2}{2m}$

Substituting value of $\Delta p \rightarrow$

$$E = \frac{(0.527 \times 10^{-20})^2}{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19}}$$

$$= 97 \text{ MeV}$$

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In experimental observations, the maximum kinetic energy of electron is found to be nearly 4 MeV. So having an energy of order 97 MeV is not possible, which proves that electrons does not exist in nucleus.

② Existence of protons in nucleus.

From Heisnberg's uncertainity principle we have,

$$\Delta x \cdot \Delta p = \frac{h}{4\pi}$$

Now, if proton exists inside the nucleus, the maximum uncertainity in its position will be of order of diameter of nucleus, i.e, $\Delta x \simeq 10^{-14}$ m.

Substituting Δx, we get -

$$10^{-14} \cdot \Delta p = \frac{h}{4\pi}$$

$$\Rightarrow \Delta p = \frac{6.626 \times 10^{-34} \text{ J-s}}{4 \times 3.14 \times 10^{-14} \text{ m}}$$

$$\Rightarrow \Delta p = 0.527 \times 10^{-20} \text{ kg m/s}$$

We know, kinetic energy, $E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$

Substituting $\Delta p \Rightarrow E = \frac{(0.527)^2 \times (10^{-20})^2}{2 \times 1.67 \times 10^{-20} \times 1.6 \times 10^{-19}}$

$$= 52 \text{ KeV}$$

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This value of kinetic energy is smaller than the energies of the particles emitted by the nucleus. Hence protons does exist inside the nucleus.

Dual Nature of Matter [De-Broglie Hypothesis]

According to De-Broglie, every moving particle exhibits wave nature. The wave associated with a particle moving with velocity v is given as-

$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

λ is wavelength.

Wave particle duality

All energy in universe exists in form of radiation and matter. Since nature exhibits a fundamental symmetry. If radiation behave as both waves and particle, so matter as well can show particle as well as wave properties.

Matter Waves properties

The waves associated with moving matter are known as matter waves. There properties are-

① The wavelength of these waves is given by $\lambda = \frac{h}{mv}$, where v is velocity and m is mass.

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② Matter waves are localized waves [finite in space] and are not progressive waves [infinite spread].

③ Matter waves are not single waves. They are group of waves, known as wave packet.

④ Matter waves represent the direction of propagation of matter.

Different forms of De-Broglie Formula:

① For a particle having Kinetic energy

We have, $\lambda = \frac{h}{mv}$ ← (5)

Also $K.E = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m}$ ← (6)

$\Rightarrow m^2v^2 = 2m(K.E.)$

$\Rightarrow mv = \sqrt{2m(K.E)}$

Substituting in (5) →

$$\lambda = \frac{h}{\sqrt{2m(K.E.)}}$$

Where m is mass of given particle.

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② For a charged particle in potential (V^e)

We know, $\lambda = \frac{h}{mv}$

Also from equation 6, $K.E = \frac{1}{2}\frac{m^2v^2}{m}$

For a charged particle kinetic energy, $K.E = eV$

(where e is charge and V is voltage)

Equating both kinetic energies —

$$\frac{m^2v^2}{2m} = eV \quad \left[\begin{array}{l}\text{small v is velocity}\\ V \text{ is voltage}\end{array}\right]$$

$$\Rightarrow mv = \sqrt{2meV^e}$$

Substituting, $\boxed{\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2meV}}}$

③ For a particle in thermal equilibrium at T,

The kinetic energy for a thermal particle $= \frac{3}{2}K_BT$

(where K_B is Boltzmann constant)

Also from, Equation 6, $K.E = \frac{1}{2}\frac{m^2v^2}{m}$

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Equating both energies -

$$\frac{1}{2m} \times m^2v^2 = \frac{3}{2} k_B T$$

$$\Rightarrow mv = \sqrt{3mk_BT}$$

Substituting → $$\boxed{\lambda = \frac{h}{mv} = \frac{h}{\sqrt{3mk_BT}}}$$

Group Velocity and Phase Velocity

The velocity with which the wave-packet which is formed due to the superposition of two or more waves of slightly different wavelengths is transmitted is known as group velocity. It is represented as

$$\boxed{v_g = \frac{dw}{dk}}$$ [where w is angular frequency]

→ [here k is wave number defined as $k = \frac{2\pi}{\lambda}$]

The individual velocity with which a individual wave in wave packet is transmitted is known as phase velocity. It is given as

$$\boxed{v_p = \frac{w}{k}}$$

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Relationship between group and phase velocity

From definition of phase velocity, we have -

$$v_p = \frac{\omega}{k}$$

$$\Rightarrow \omega = k . v_p$$

Differentiating both sides with respect to $k \rightarrow$

$$\frac{d\omega}{dk} = v_p \frac{dk}{dk} + k \frac{dv_p}{dk}$$

We know $\frac{d\omega}{dk} = v_g$

$$\text{So} \Rightarrow \quad v_g = v_p + k \frac{dv_p}{dk}$$

Using partial differentiation -

$$v_g = v_p + k \frac{dv_p}{d\lambda} \frac{d\lambda}{dk} \leftarrow (1)$$

We know that, $k = \frac{2\pi}{\lambda} \Rightarrow \lambda = \frac{2\pi}{k}$

Diff. w.r.t $k \longrightarrow$

$$\frac{d\lambda}{dk} = -\frac{2\pi}{k^2}$$

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Substitute value of $\frac{d\lambda}{dk}$ in (1) $\rightarrow$

$$V_g = V_p - \frac{2\pi}{k}\frac{dV_p}{d\lambda} \quad \left[\frac{2\pi}{k} = \lambda\right]$$

$$\Rightarrow \boxed{V_g = V_p - \lambda\frac{dV_p}{d\lambda}}$$

This gives relation between V_g and V_p.

Wave function

In quantum mechanics, the wave function $\Psi(x,y,z,t)$ is a mathematical function that completely describes the quantum state of a particle.

Physical Significance of wave function

The wave function $\Psi(x,y,z,t)$ does not have any physical significance of its own. The modulus square of wave function, i.e, $|\Psi(x,y,z,t)|^2$, known as probability density gives the probability of finding the particle at that position and time.

$$|\Psi(x,y,z,t)|^2 = \Psi^*\Psi$$

where Ψ^* is the complex-conjugate.

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→ This interpretation of $|\psi|^2$ was given by Max Born.

Properties of Wave function

① In order to avoid infinite probabilities, ψ must be finite for all values of x, y, z.

② In order to avoid multiple values of probability, ψ must be single valued for all x, y, z.

③ The first order derivatives of ψ, i.e, $\frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial z}$ must be continuous in all regions.

④ The wave function must obey normalization condition, that is,

$$\int_{-\infty}^{\infty} |\psi(x,y,z,t)|^2 dx\,dy\,dz = 1$$

⑤ In order to normalize the wave function, ψ must approach zero as x, y, z, approaches infinity.

Important formulas

① $E = h\nu$ [E is energy, h is planck's constt., ν is frequency]

② $E = \frac{hc}{\lambda}$ [c is speed of light, λ is wavelength]

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③ $\Delta x \cdot \Delta p = \frac{h}{4\pi}$

④ $\Delta E \cdot \Delta t = \frac{h}{4\pi}$

⑤ $\lambda = \frac{h}{mv}$ [m is mass, v is velocity]

⑥ $\lambda = \frac{h}{\sqrt{2m(K.E.)}}$ [K.E is kinetic energy]

⑦ $\lambda = \frac{h}{\sqrt{2mqV}}$ [q is charge, V is voltage or potential difference]

⑧ $\lambda = \frac{h}{\sqrt{3mK_BT}}$ [T is temperature, K_B is boltzmann constant]

Important Constant

① Planck's constant (h) = 6.626×10^{-34} J.sec

② Mass of electron (m_e) = 9.31×10^{-31} kg

③ Mass of proton (m_p) = mass of neutron = 1.67×10^{-27} kg

④ Boltzmann's Constant (K_B) = 1.38×10^{-23} J/K

⑤ Charge on electron and proton = 1.6×10^{-19} C

⑥ Speed of light (c) = 3×10^{8} m/sec

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